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**Electrochemical simulation of three novel cardiovascular drugs phase I metabolism and development of a new method for determination of them by liquid chromatography coupled with tandem mass spectrometry**

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**Abstract**

In this study electrochemistry (EC) coupled with electrospray ionization mass spectrometry (ESI-MS) was used to study the metabolic fate of three novel cardiovascular drugs: rivaroxaban (RIV), aliskiren (ALS), and prasugrel (PRS). Mimicry of the oxidative phase I metabolism was achieved in a simple amperometric thin-layer cell equipped with a boron-doped diamond (MD) working electrode. Structures of the electrochemically-generated metabolites were elucidated from MS/MS experiments. Additionally, a sensitive, specific, and rapid ultra-high performance liquid chromatography–tandem mass spectrometer (UHPLC–MS/MS) method has been developed and validated for the selected drugs in human urine samples. Three different sample preparation methods were compared and finally, sample preparation was accomplished through an ultrasound-assisted emulsification microextraction process (USAEME). The drugs were detected using a triple quadrupole tandem mass spectrometer by multiple reaction monitoring *via* an electrospray ionization source with positive ionization mode (ESI(+)). The results obtained by EC–MS were compared with conventional *in vivo* studies by analyzing urine samples from patients. Data from *in vivo* experiments showed good agreement with the data from electrochemical oxidation. Thus, EC–MS is very well-suited for the simulation of the oxidative metabolism of rivaroxaban, aliskiren, and prasugrel as well. Moreover, electrochemical conversion of target compounds appears to be a new *in vitro* technology for the prediction of potential metabolites.

**Keywords:** Cardiovascular drugs; liquid chromatography; electrochemistry; extraction; mass spectrometry

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